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CRYSTALLINE STRUCTURE OF ALKYL HALIDES OF MERCURY

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[A Digest]

Members of a homologous series of normal alkyl halides of mercury -- CH_3HgCl, C_2H_5HgCl, C_2H_5HgBr, C_3H_7HgCl, and C_4H_9HgCl -- were subjected to X-ray analysis for the first time. Their spatial groups, D_{4h}^1 - P/nmm, (and for C_4H_9HgCl, C_{2v}^1 -Pmn) and dimensions of their elementary configurations were determined to be as follows: CH_3HgCl - a = 4.62 A, c = 9.39 A; C_2H_5HgCl - a = 4.65 A, c = 10.82 A; C_2H_5HgBr - a = 4.90 A, c = 10.62 A; C_3H_7HgCl - a = 4.70 A, c = 13.62 A; C_4H_9HgCl - a = 4.10 A; b = 5.34 A; c = 15.16 A.

In the tetragonal crystals, the atoms of mercury and chlorine, and also the centers of the radicals lay on the fourth axis. Coordinates of the mercury atom in the cell were found to be 1.30, 1.31, 1.28, 1.33, and 1.28 A, respectively.

From the electron densities for CH_3HgCl, C_2H_5HgCl, and C_2H_5HgBr, the interatomic interval for Hg - Cl and Hg - Br was calculated at 2.50 A, and for Hg - C at 2.06 A. The latter figure was obtained by X-ray analysis for the first time. The margin of error in these computations was plus or minus 0.03 A.

The free, but coordinated rotation of the CH_3-, C_2H_5-, and C_3H_7- group and the lack of rotation of the C_4H_9- group were shown geometrically and with X-rays, and effective radii of rotation determined. The intermolecular radius of the mercury was found to be 1.50 A.

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The crystalline structure of mercury alkylhalogenides.

by

D.R. Grdenich and A.I. Kitaigorodskii

1. Introduction

Up to the present time not one work has been dedicated to the study of the crystalline structure of the mercurial organic compounds. Study on the salts of mercury and mercury alkyl mercaptans have been carried out by the Röntgen method. The results of these works give sufficiently unassuming knowledge relative to the inter-atomic and inter-molecular intervals (Translator's note: The Russian word can be translated either interval or space throughout the entire article.) Several works are dedicated to the crystalline structure of mercury cyanide, and the structure of it is finally explained by Zhdanov and Shugam (1). They establish the fact that the molecule has a linear configuration not adduced from any data relative to the mercury-carbon interval.

The inter-atomic interval C-Hg is known from basic electron-graphic study of dimethylmercury vapor - 2.20 A (2) and dipara-bromphenyl mercury - 2.10 A (3).

The reason for so few works in this field is explained by the difficulty of studying mercury compounds. The mercury atom possesses many large dispersions which are capable of being compared with the light atoms, and precise determinations on the position of the latter along with the mercury atoms are assumed to be hardly possible. Thus, for example, in the work on the study of the crystalline structure of the mineral aglestonite Hg_4Cl_2O (4) it is pointed out that the position of the atoms of chlorine and oxygen is impossible to be determined because its dispersion capacity is very poor. From all this it is seen that the organic compounds of mercury remain beyond the attention of the student, because they are an "ungrateful" ("thankless"?) object of röntgen-structural analysis.

On the other hand the study of the chemical behavior of the mercury organic compounds has developed in rapid steps. From the work of A.N. Nesmeyanov, R.K. Freidlina, A.E. Borisov and their collaborators (5) is explained a complete series of questions concerning the nature of the mercury organic compounds and the product of addition of mercury salt with indefinite compound discoveres a new type of compound - a quasicomplex.

Studies of the crystalline structure of certain quasicomplexes of mercury organic compounds are adduced by A.I. Kitaigorodsky (6).

He has indicated in what extent it is necessary to have accurate knowledge on the mercury-carbon interval. The present work has been begun for this purpose. For the object of study we have taken mercury alkylhalogenides.

II. Crystalline structure of mercury alkylchloride

In the chemical literature a homologous series of normal mercury alkyl chlorides, bromides and iodides is described with the carbon number in the chain from 1 to 7 and at 16.(7). We have taken the methyl-, ethyl-, propyl- and butylchlorides for study.

A. Mercury methyl-, ethyl- and propyl-chloride. Crystals of the compounds CH_3HgCl, C_3H_7HgCl and C_2H_5HgCl have been studied by physical methods up to the present time. They belong to the tetragonal system as we established according to a "Lauegram" (Translator's note: this is a transliteration of the word) (Lauevsky class of symmetry D_{4h}) and according to the Röntgengram of oscillation. The study of similar polarized light indicates that these crystals have one axis. All the crystals are represented by a transparent, very thin (with average thinness of 0.002 cm), broad plate (up to 2 cm^2 in area) with irregular contours. The measurement of the elementary nucleus is determined according to the Röntgengram of Oscillation, but afterwards the measurement is made more precise by the ionization spectrometer.

CH_3HgCl	C_2H_5HgCl	C_3H_7HgCl
a = 4.62 A	a = 4.65 A	a = 4.70 A
c = 9.59 A	c = 10.82 A	c = 13.62 A

(The direction of axis c is perpendicular to the plane of the plate.) Because for the density for CH_3HgCl rho equals 3.83 and for C_2H_5HgCl rho equals 3.482 (8), then in the nucleus of these compounds there are two molecules. In the nucleus of C_3H_7HgCl there are two molecules because in the calculation of density rho is 3.06.

By the method of the inverted lattice there is indicated a series of Röntgengrams of oscillation and it is found that they are all reflexes with indices hkl, all oool, but extinction hko, with uneven amount h plus k. By such law of liquidation it possesses C_{4h}^3 - P 4/n group but it drops off because the Lauegram indicates a higher symmetry. The group of the C_{4v} class also drops off, because it is indicated that there is an axis of the fourth order and perpendicular to it a sliding plane.

There remains the group of the D_{4h} class. By the law of liquidation it satisfies the D_{4h}^7 - P 4/nmm group with individual position for the mercury, chlorine and carbon atoms (00_z) and $(1/2\ 1/2\ \bar{z})$.

From the measurement of the nucleus and the arrangement of the elements of symmetry it is seen that the atom might be placed only in the axis c, that is, in the axis of the fourth order. Because the same molecule does not possess this symmetry, then it is necessary to suppose thatthe alkyl group is capable of being rotated in the lattice around the mercury-carbon chain. Similar rotation of a molecule or part of a molecule in the crystalline lattice is already established in the measurement of the compound with alkyl groups (9). The question of the possibility of similar rotation of alkyl groups of compounds studied by us is examined below.

The crystalline structure found explains the physical property of the crystals of these compounds, for example, cleavage of the complete plate, volatility, and form of the crystals.

The parameter z_{Hg} might be defined from the determination of intensity of the reflex ool according to the Röntgengram of oscillation. Accurate determination is produced by measurement of the intensity by the ionization method. Disregarding at first the influence of the proximity of the chlorine and carbon atoms in dispersion, we introduce an insignificant error.

In table 1-3 and in illustration 3 is seen that the significant structure of the amplitude (structure of amplitude

$A = 2 \cos 2\pi \left(\frac{h + k}{4} + lz\right)$ has the form $A = 2 \cos 2\pi lz$ for the reflex ool; the beginning coordinate in the center of symmetry). The results obtained are:

CH_3HgCl: $z_{Hg} = 1.30$ A

C_2H_5HgCl: $z_{Hg} = 1.31$ A

C_3H_7HgCl: $z_{Hg} = 1.33$ A

b. Crystalline structure of mercury butylchloride. The crystal of C_4H_9HgCl possesses for example the same form, but does not grow as rapidly. In similar polarized light it gives a picture typical for the bi-axial crystals. The Lausgram, taken perpendicular to the plate, indicates the symmetry D_{2h}. The crystals consequently appeared to be rhombic. The elementary nuclei are determined according to the Röntgengram of oscillation; such periods along the basic direction (from axis c acceptance of the normal to the plane of the plate):

a = 4.10 A b = 5.39 A c = 15.16 A.

The density is roughly determined ar rho = 3; thus the number of molecules of the elementary nuclei z = 2 (calculated at 2.07).

We have carried out the Röntgengram oscillation and found the following reflex: hkl all, hol all, okl all, and hko only ch + k = 2n. The spatial group is chosen on the basis of the

following reasoning. At first the holohedral class D_{2h} is rejected because it is difficult to suppose a similar rotation of the butyl group around the axis of the second order. Such a supposition is confirmed by study on the structural - investigation, concerning which we have an outline below. According to this same reason the class D_2 drops off. There remains class C_{2v} which is found by liquidation and by geometric requirements to satisfy the group C_{2v}^7 - Pmn (plane n perpendicular to the axis c) with the position of the mercury atom in points oyz; $(1/2 + 1/2\ \bar{z})$. Consequently the molecule C_4H_9HgCl is found in the plane of symmetry. This is undoubtedly plane (100) because b a.

A complete study of the structure is not carried out. There is determination only of the parameter of mercury z_{Hg} with the aid of the evaluation of the intensity reflex ool by Röntgengram of oscillation and the ionization method. The dependence of the structural amplitude on z is given in table 3. Disregarding the presence of the light atoms (here the error is greater) we obtain z_{Hg} = 1.26 - 1.30 A (because the reflex 003 is exceptionally weak).

From this it is seen that the relative position of the mercury atom in the lattice is not changed in the chloride series from methyl- to butyl-.

III. Inter-atomic intervals Hg-C and Hg-Cl

Determination of the coordinates of the mercury, chlorine and carbon atoms of the crystals studied is significantly facilitated by the fact that all the atoms are found in a straight line. Expediently the construction projection of the electron density is on the plane (010)

$$\text{rho}\,(xz) = \frac{1}{2c} \sum_{h} \sum_{l} F_{hol} \cos 2\pi \left(h \frac{x}{a} + l \frac{z}{c}\right.$$

The sign F_{hol} is determined by coordinates of mercury atom known by us. The measurement of the reflex is carried out on ionization spectrograph. Altogether 40 reflexes are measured (of 55 possible from the conditions of our experiment, applying the curve K_a -Cu). The ratio of the least to the greatest measured intensity equals 1: 250.

The factor of absorption plays the greatest role, because the coefficient of absorption mu = 800 for CH_3HgCl (experimentally determined) and mu = 590 for C_2H_5HgCl. It is calculated for each reflex according to the formula:

$$A = \frac{2}{2\mu} \frac{\sin(2\theta + \text{alpha})}{\cos(\theta + \text{alpha})\sin\theta} \left[e^{\frac{-z_0\mu}{\sin(\theta + \text{alpha})}} - e^{\frac{-z_0\mu}{\sin \text{alpha}}} \right]$$

where s = the size of the groups, alpha = the angle of the falling of the rays from the plate, z_0 = the thickness of the plate but θ = the "breggovsky" angle.

In the tables are given the calculations and measurements of the amplitudes of F_{hol}. The definite significance of F measured is, for example, for the reflex 103, 104, 105 for which the angle alpha is small ($\sim 5°$) and the formula gives an inaccurate significance for A (the formula is accurate for a limitless plate).

A significant role is played by the temperature factor. The reflex of a distant series 30 ell + 50 ell is not observed either in Röntgengram or in spectrograph. The temperature factor increases from methyl to ethyl and propyl chloride so that it is possibly found in relation to the independent rotation of the alkyl group. In C_2H_5HgCl there is observed a still smaller number of reflexes (35). The temperature factor $e^{-B\left(\frac{\sin\theta}{\lambda}\right)^2}$ for methylchloride is given with the value B = 4.

The value of the function rho (xz) is calculated for the period taken across 1/48 period. The curve of distribution of electrons for CH_3HgCl and C_2H_5HgCl is along the direction (001), that is, along the axis of the molecule given in illustrations 2 and 3; it is clearly seen that the interval of atoms might be sufficiantly

accurate to determine because the maximum is clear and sharp (even the maximum belonging to carbon).

The coordinate of the maximum is defined approximately by the function obtained in the region of the maximum curve of the third order (not by graphic but by analytical method). The coordinates obtained are:

CH_3HgCl: $z_{Hg} = 1.30$ A

$z_C = 3.36$ A

$z_{Cl} = 1.20$ A

C_2H_5HgCl: $z_{Hg} = 1.31$ A

$z_{Cl} = 1.21$ A

The interval of Hg-C (of CH_3HgCl): $z_C - z_{Hg} = 2.06$ A, but the interval Hg-Cl: $z_{Hg} - z_{Cl} = 2.50$ A.

A number similar to that for Hg-Cl is obtained for C_2H_5HgCl.

The interval of Hg-C = 2.06 A obtained by us according to my results to close to that obtained by electronographic means.

The interval Hg-Cl = 2.50 A does not coincide with the literature data - 2.25 A is obtained from definite structure of the mercuric bichloride (10). This value (2.25 A) is obtained by the authors by indirect means and may not be claimed to be authentic.

Not completely authentic either is the number 2.36 A which is given for the interval Hg-Cl in the chlorethyl mercaptan of mercury (11).

Up to this work the interval Hg-Cl has been determined electronographically (12). For the mercury bichloride vapor the number 2.20 A is adduced.

In such a way up to the present time we not only do not have a definite value for the Hg-C bond but also there is contradiction in relation to the value of the length of the Hg-Cl bond.

There is a single work where the value of 2.50 A has been determined for the Hg-Cl bond - this is the work of Havighurst (13). This author studied the crystalline structure of calomel Hg_2Cl_2 and also Hg_2Br_2 and Hg_2I_2. In application of the photographic and ionization methods one constructs a series of electron densities (one of the first Fuhr series of structural analysis) and obtains the maximum belonging to mercury and halogen. The value obtained in this way might be stated as the most accurate and objective. For the interval Hg-Br the value 2.56 A is adduced.

For testing the results of our preceding studies we took the mercury ethylbromide. This compound is isomorphic with the ethylchloride which has been verified by conoscopic study and

Röntgengram oscillation. The measure of the elementary nuclei is: a = 4.90 A, c = 10.62 A. The period along the axis a is increased in conformance with the increased radius of the bromine atom in comparison with the radius of the chlorine atom. It is interesting that the period along the length of the mercury ethylbromide molecule is less in 0.20 A than in C_2H_5HgCl which explains a more profitable "wrapping up."

By the ionization method the intensity of reflex hol for C_2H_5HgBr is measured (table 4). 24 reflexes are found and the construction series of electron densities are as those for C_2H_5HgCl and CH_3HgCl. The curve of distribution of the electron density along the direction (001) is given in illustration 4.

The coordinates of the atom are the following: z_{Hg} = 1.28 A, z_{Br} = 1.23 A, which gives the interval Hg-Br: $z_{Hg} + z_{Br}$ = 2.51 A.

Equal values for the intervals of Hg-Cl and Hg-Br may be established within the limits of error.

In his work on the study of the structure of mercury trans-chlorvinylbromide A.I. Kitaigorodsky cites the interval Hg-Br = 2.43 A. In such a degree registration of the Hg-Br interval in the given compound is completely comprehensive if we take into account the fact that the mercury atom acquires a

positive charge, attracting it to the bromine atom, in consequence of the superposition of the complex and normal structure (5).

We have basis to doubt the accuracy of the determination of the Hg-Cl interval in mercuric bichloride, especially since it is proposed by some authors (10) that the intermolecular interval Cl-Cl in layers, the length of the Hg-Cl bond and the turning of the molecule also may change.

The curve of distribution of the electron density in C_2H_5HgCl and C_2H_5HgBr gives the position of the carbon atom much less clearly than in CH_3HgCl. This is explained previously in all by the fusion of two carbon atoms in projection and also by the fewer number of reflexes taken for construction of the series, and by the free rotation of all the ethyl groups. Two carbon atoms may not be permitted and the distribution of their electrons should be poured off in a series of one diffused maximum. This maximum appeared to be the center of the $CH_2 \cdot CH_3$ group. In the projection of the $CH_2 \cdot CH_3$ the interval equals 0.5 A. Thus the interval from the mercury atom to this maximum ought to be 0.25 A more than to the nearest carbon atom. The experiment points out that this interval really is of the order of 2.3 - 2.5 A.

IV. Free rotation and intermolecular interval

The possibility of free rotation of the molecule in crystalline lattice is indicated by Pauling (8). Pauling bases his supposition on a complete series of facts, among them, on the symmetry of the lattice. When the molecule occupies a special position in the lattice, that is, rests on some elements of macrosymmetry, then it should possess this symmetry. First, it would seem that a violation of this law is observed in crystals of alkyl ammonium salts (9 a). This fact is pointed out then somewhat strangely, that is, it introduced a supposition of the alkyl group (9 a, c). Pauling indicates that the inertia of such a chain around the axis along this chain is somewhat small, so that free rotation is completely possible even at room temperature. Such a rotated molecule possesses symmetry of the cylinder, that is, includes in itself an axis of the preferred order.

In our cases the free rotation of the methyl, ethyl and propyl group is demonstrated, bythe Röntgen method. In spite of this the demonstration of this fact is possible and by geometric means with the aid of structural investigation (Concerning the method of geometric analysis see (14)).

The alkyl group of the molecule, related to relaying along axis a, is concerned with favorable rotation. After this is considered

the alkyl group related by symmetrical operation, namely relation of the alkyl group in position (00_z) with alkyl group in (1/2 1/2 c-z). At the same time as the chlorine atom is related to the mercury atom, the tangency is lacking. Consequently on one side we have the possibility of defining the effective radius of the rotating alkyl group, but on the other side, of verifying the significance of the intermolecular radius of mercury atom, taking into account the intermolecular radius of mercury atom, taking into account the intermolecular radius of chlorine 1.8 A and bromine 1.95 A.

The interval, in which we found the mercury atom and the chlorine atom in the neighbouring molecule, equals:

$$r_{Cl} + r_{Hg} = \sqrt{(Z_{Hg} - Z_{Cl})^2 + \frac{a^2}{2}}$$

For r_{Hg} the following value in crystals is found

CH_3HgCl $r_{Hg} = 1.48$ A

C_2H_5HgCl $r_{Hg} = 1.52$ A

C_2H_5HgBr $r_{Hg} = 1.52$ A

For rotating the methyl group the intramolecular radius is obtained:

$$r_{CH3} = 1/2\sqrt{(C - 2Z_c)^2 + \frac{a^2}{2}}$$

for CH_3HgCl: $r_{CH3} = 2.11$ A.

The given value in 0.1A is less universally adopted. For justifying these values, both here and also in the ethyl and prop. groups we ought to accept the supposition on the coordinated rotation. For example in the lattice of CH_3HgCl the simultaneous pivot of the two related methyl groups of the hydrogen atoms towards each other is impossible without significant alteration of the intermolecular interval.

For this same reason the ethyl groups of the neighbouring molecule of mercury ethyl chloride may not simultaneously be found in the plane (110) because in this case the hydrogen atom is found in an interval of 3.10 A, which is less than the intermolecular diameter of hydrogen of 3.4 A. Consequently the ethyl groups passed each other by. Their methyl groups rotated in coordinate manner. The same occurs in propyl chloride.

The ethyl and propyl groups of the molecule, related to period a, also might rotate only in coordinate manner. In this case their effective radius equals $\frac{a}{2}$ that is 2.35 A.

The possibility of free rotation of the butyl group in mercury butyl chloride is rejected by geometric analysis. The butyl groups are found in plane (100) appearing as planes of symmetry. Although the butyl group on the whole does not rotate, the free rotation of the CH_3 group is possible without violation of the laws of symmetry. The size of the phase a = 4.10 A gives

the possibility for the C_4H_9 group for oscillating around the direction of the C-Hg bond.

The study of the structure of the higher members of the series is not of special interest. Its structure is to be the same as the structure of butyl chloride. In figures 5 and 6 is given the "packing up" of the molecule of methyl and propyl chloride.

V. Experimental part

The preparation of our compounds C_2H_5HgCl, C_2H_5HgBr, C_3H_7HgCl and C_4H_9HgCl according to the method of Slotta and Jacobi (7) is subject to purification by means of crystallization from ethyl alcohol and benzol, since then for the time being, a suitable point of fusion has not been attained. The culture of the crystals is carried out by slow precipitation of saturated alcohol solution.

The orientation of the crystals in rontgen chamber cell is carried out according to Lausgram. Methyl-, ethyl- and weakly propyl-chloride mercury compounds, sublimated at room temperature. The measurement on one crystal might be conducted in this case only if we surround the crystal with a cylinder of cellphane, placed within some crystals of the same substance. In this way we are guaranteed the saturation of the space in which the object is found, and its own vapor.

Plates, analogous to mica, possess remarkable cleavage. In the majority of cases the separate layers of the plate are turned relatively on each other and give diffused spots on the Lauegram. Consequently this property of choice and orientation of objects for exposure and measuring in spectograph is difficult in significant measure. The measurement of relative intensity is carried out by the ionization method with the aid of the spectrograph. The strengthening of the ionization current is carried out with the aid of the pliotron scheme, and the current is measured by mirror galvanometer with the sensitivity $1.2 \cdot 10^{-8}$ A in one graduation scale.

Copper radiation has been used. The intensity of light is regulated with the aid of the current from an incandescent tube. The dependence of the indicated galvanometer on the current in the tube is linear for all the measurements bands.

VI. Accuracy of the experiments and calculations

Because the atoms, molecules and compounds studied are situated in one direction - along (001), the accuracy of definition of the interatomic interval of the first order depends on the accuracy of the definite period along axis c. This period is defined by numerous measurements in a few samples of angle of divergence for the distant reflex ool (to 008). This period

is ...ined for CH_3HgCl with the aid of the stectrograph (on 3 objects) and is taken from 25 values on the average 9.39 A with probable quadratic error of 0.013 A. In relation to the limit of error we might affirm that in some cases it does not exceed ± 0.04 A. Such an average value is obtained by us by the Debye method (radius of the chamber 43 mm).

Period c is defined with such an accuracy for C_2H_5HgCl and C_2H_5HgBr. The probable quadratic error in the first case in the average value of the period 10.82 A (for C_2H_5HgCl) equals 0.01 A but in the second - still less.

The period of identity in the plane of the plate (a) is defined with somewhat less accuracy, because in the case of CH_3HgCl and C_2H_5HgCl might be found only reflex 200 and 400, but in the case of C_2H_5HgBr only 200. This period in the case of CH_3HgCl is defined according to Röntgenogram oscillation, on the spectrgraph and the method of powder. The result obtained is 4.62 A with maximal dispersion of 0.08 A.

Conversion to accuracy of definite coordinate atoms. As is pointed out above, coordinates of atoms are determined from the F_{hol} - interpolation series. The error of interpolation is insignificant, because the value of dispersion obtained does not ± 0.01A.

The value of F_{hol} taken in a series (of arbitrary units) is determined on the average with error of 10%. Consequently from the formula

$$r = 0.707 \cdot 0.1 \sqrt{\sum_{i=1}^{40} F_i^2} \qquad (15)$$

is obtained the error of the sum of the series as r = 6 (of the same units). The error is defined with corrdinates maximum Δ_z related with value r, with acuteness of maximum and size of the interval period, through which is calculated the value of the function $\rho(xz)$ (in our case 0.1955 A for CH_3HgCl). For coordinates' of mercury (for CH_3HgCl) $\Delta_z = 0.005$ A, for carbon $\Delta_z = 0.02$ A and for chlorine $\Delta_z = 0.02$A.

Taking into consideration the error in definite period it might be supposed that the interatomic interval obtained by us is defined with accuracy of $\pm$ 0.03 A.

Summary

1. First is studied by the Röntgen method a homologous series of normal mercury alkyl halogenides: CH_3HgCl, C_2H_5HgCl, C_2H_5HgBr, C_3H_7HgCl and C_4H_9HgCl. The determination of spatial group (D_{4h}^7 - P/mmm and for C_4H_9HgCl C_{2v}^7 - Pmm) and measure of the elementary cell.

CH_3HgCl	C_2H_5HgCl
a = 4.62 A	a = 4.65 A
c = 9.39 A	c = 10.82 A
C_2H_5HgBr	C_3H_7HgCl
a = 4.90 A	a = 4.70 A
c = 10.62 A	c = 13.62 A
C_4H_9HgCl	
a = 4.10 A	
b = 5.34 A	
C = 13.16 A	

2. In tetragonal crystals the atoms of mercury and chlorine and also the center of the radical rests on the fourth axis. The corrdinates of mercury atom in the nuclei is shown as the following:

CH_3HgCl	C_2H_5HgCl
z_{Hg} = 1.30 A	z_{Hg} = 1.31 A
C_2H_5HgBr	C_3H_7HgCl
z_{Hg} = 1.28 A	z_{Hg} = 1.33 A
C_4H_9HgCl	
z_{Hg} = 1.28 A.	

3. From a series of electron densities for CH_3HgCl, C_2H_5HgCl and C_2H_5HgBr is obtained interatomic interval: Hg-Cl and Hg-Br 2.50 A, Hg-C 2.06 A.

The Hg-C interval is defined by the Röntgen method first. The adduced value is obtained with accuracy of $\pm$ 0.03A.

4. By the Röntgen and geometric method it is indicated as free but coordinate rotation of CH_3-, C_2H_5 and C_3H_7 groups in lattice and absence of rotation in the C_4H_9 group. The determination is effective for the radius rotation. The intermolecular rotation of mercury is indicated as equals 1.50 A.

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